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OAK RIDGE SCHOOL OF REACTOR TECHNOLOGY

Multigroup-Multiregion Theory for the Consistent
 P_1 Approximation to the Boltzmann Equation

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OAK RIDGE SCHOOL OF REACTOR TECHNOLOGY

F. C. Vonderlage, Director

CF-55-8-189

"MULTIGROUP-MULTIREGION THEORY FOR THE CONSISTENT P_1 APPROXIMATION
TO THE BOLTZMANN EQUATION

B. JOHN GARRICK

AUGUST 1955

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PREFACE

In September, 1954, a group of men representing various scientific and engineering fields embarked on the twelve months of study which culminated in this report. For nine of these months, formal classroom and student laboratory work occupied their time. At the end of that period, this student was presented with a problem in reactor design.

This is a summary report of the study, the research, the problems and the solutions which developed during the final ten-weeks period of the school term. It must be realized that, in so short a time, a study of this scope can not be guaranteed complete or free of error. This "thesis" is not offered as a polished engineering report but rather as a record of the work done by this student under the leadership of the advisor. It is reproduced for use by those persons competent to assess the uncertainties inherent in the results obtained in terms of the preciseness of the technical data and analytical methods employed in the study. In the opinion of the student and faculty of ORSORT, the problem has served the pedagogical purpose for which it was intended.

As a matter of historical fact and pride we point out that similar investigations by student groups of previous ORSORT classes have led to sufficiently encouraging results to warrant more exhaustive studies; in at least one instance, a reactor first investigated by a student group is soon to become a physical reality. There is also recorded an instance in which calculations contained in a similar report were uncritically abstracted and applied to a study for which they were never intended. It is to avoid the recurrence of the latter experience that we have taken some pains to acquaint the reader with the character of this report.

The faculty wishes to join the author in an expression of appreciation for the assistance which various members of the Oak Ridge National Laboratory have so generously contributed. In particular, the guidance of the consultant, Robert R. Coveyou, is gratefully acknowledged.

F. C. VonderLage
for
The Faculty of ORSORT

ACKNOWLEDGMENT

Acknowledgment is made to R. R. Coveyou for the development of the method contained in this report. Appreciation is expressed to R. R. Bate for his helpful advice and criticism. Special acknowledgment is also extended to W. E. Kinney for his guidance and service rendered. Had it not been for his efforts, preparation of this report in the allotted time would have been impossible.

ABSTRACT

The consistent P_1 integral equations in lethargy and space, together with the coupling equations expressing the slowing down of neutrons, are reduced to a set of partial differential equations describing the P_1 approximation.

The group equations are integrated over lethargy by assuming flux linearity over a lethargy interval. Consideration is given to the thermal motion of the moderator atoms in developing the thermal group equations and their distribution of velocity is assumed Maxwellian as it is for the neutrons.

The spatial integration is performed by approximating the differential equation by a difference equation and integrating utilizing a technique developed by A. H. Fox.

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INTRODUCTION

The theory reported herein is a multigroup-multiregion technique for application to criticality and related reactor computations. Of particular interest is the fact that the method developed is suitable for hydrogen as well as for heavier moderator systems. It also describes the neutron physics near boundaries more accurately than ordinary diffusion theory.

The method is based on the consistent P_1 approximation to the Boltzmann equation; i.e., the angular distribution of neutrons is represented by the first two terms in the spherical harmonic expansion. Two slowing down equations are defined on the basis of an isotropic scattering kernel and an angular scattering kernel. By use of a Taylor series expansion the integral slowing down and P_1 equations are expressed as a set of partial differential equations. Since these equations take on simple solutions for heavy moderators, three classes of elements were defined in Section II.

The basic assumption for development of the group equations from the differential equations is one of flux linearity over a lethargy interval. The group constants are then expressed in terms of the lower endpoint and midpoint flux. The constants could also have been expressed in terms of the two endpoints; however, they took on a somewhat simpler form when the above technique was used.

In treating the thermal group, consideration was given to the thermal motion of the moderator atoms as well as the neutrons. It was assumed that the neutrons and moderator atoms followed a Maxwell-Boltzmann distribution of velocity. Simplifying assumptions were also made on

the scattering kernels.

To perform the spatial integration, a difference equation was sought which would more accurately approximate the differential equation. The difference equation was then integrated by a method due in principle to A. H. Fox.

The theory developed in this report is to serve as a basis for a multigroup-multiregion code presently being prepared for use on the ORACLE.

MULTIGROUP-MULTIREGION THEORY FOR THE CONSISTENT P_1
APPROXIMATION TO THE BOLTZMANN EQUATION

I. DEVELOPMENT OF THE GENERAL DIFFERENTIAL EQUATIONS

The equations resulting from the consistent P_1 approximation to the Boltzmann equation are

$$\frac{1}{3} \nabla_0 \phi_0(\underline{r}, u) + \tau_n(u) \phi_1(\underline{r}, u) = \sum_n \int_0^u \phi_1(\underline{r}, u') \sigma_n(u') K_n(u' \rightarrow u) du' \quad (1.1)$$

$$\nabla_1 \phi_1(\underline{r}, u) = S(\underline{r}, u) - \tau_n(u) \phi_0(\underline{r}, u) + \sum_n \int_0^u \phi_0(\underline{r}, u') \sigma_n(u') J_n(u' \rightarrow u) du' \quad (1.2)$$

where

$u = \ln \frac{10^8 \text{ eV}}{E}$ = lethargy of neutron of energy E .

$\tau_n(u)$ = total macroscopic cross section at lethargy u of the n^{th} element.

$\sigma_n(u)$ = macroscopic scattering cross section at lethargy u of the n^{th} element.

$S(\underline{r}, u)$ = neutron source at lethargy u and position $\underline{r}$.

$\phi_0(\underline{r}, u)^{(1)}$ = neutron flux at the position $\underline{r}$ and lethargy u associated with the first harmonic in the spherical harmonic expansion, i.e., P_0 .

$\phi_1(\underline{r}, u)$ = neutron flux at the position $\underline{r}$ and lethargy u associated with P_1 .

(1) $\phi_0(\underline{r}, u)$ and $\phi_1(\underline{r}, u)$ have a direct physical interpretation. It can be shown that $\phi_0(\underline{r}, u)$ is the scalar neutron flux and $\phi_1(\underline{r}, u)$ is the net neutron current.

$K_n(u' \rightarrow u)^{(2)}$ angular scattering kernel for the n th element.

$J_n(u' \rightarrow u)$ = isotropic scattering kernel for the n th element.

$$\nabla_0 = \frac{\partial}{\partial r} \quad ; \quad \nabla_1 = \frac{\partial}{\partial r} + \frac{g}{r}$$

where $g = 0, 1, 2$ for a slab, cylinder or sphere.

Since the angular distribution of the flux is represented by the first two terms in the spherical harmonics expansion, it is necessary to consider the slowing down of neutrons resulting from angular as well as isotropic scattering. We therefore define

$$Q_n(r, u) = \int_0^u \phi_0(r, u') \sigma_n(u') \int_u^\infty J_n(u' \rightarrow u'') du'' du' \quad (1.4)$$

$$P_n(r, u) = \int_0^u \phi_1(r, u') \sigma_n(u') \int_u^\infty K_n(u' \rightarrow u'') du'' du' \quad (1.5)$$

where equations (1.4) and (1.5) are the slowing down densities due to isotropic and angular scattering, respectively. Equation (1.5) is referred to as the P_1 slowing down density.

Using equations (1.1) and (1.2), together with the coupling equations (1.4) and (1.5), we will seek a set of partial differential equations describing the P_1 approximation. To do this, it will be necessary to evaluate the scattering integrals in terms of $Q_n(r, u)$ and

$P_n(r, u)$. We begin by taking the derivatives of (1.4) and (1.5)

$$\frac{\partial Q_n(r, u)}{\partial u} = \phi_0(r, u) \sigma_n(u) - \int_0^u \phi_0(r, u') \sigma_n(u') J_n(u' \rightarrow u) du' \quad (1.6)$$

$$\frac{\partial P_n(r, u)}{\partial u} = \phi_1(r, u) \sigma_n(u) \bar{\mu}_{0n} - \int_0^u \phi_1(r, u') \sigma_n(u') K_n(u' \rightarrow u) du' \quad (1.7)$$

(2) For evaluation of the scattering kernels, see the appendix

where $\bar{\mu}_{on}$ is the average cosine of the scattering angle as evaluated in the appendix.

To reduce equations (1.6) and (1.7), we will assume that the collision densities are slowly varying functions over the lethargy range of integration. Consequently, it is permissible to expand $\sigma_n(u') \phi(r, u)$ in a Taylor series about u keeping only the first order terms; that is

$$\phi_o(r, u) \sigma_n(u') = \phi_o(r, u) \sigma_n(u) - (u - u') \frac{\partial}{\partial u} [\phi_o(r, u) \sigma_n(u)] + \dots \quad (1.8)$$

$$\phi_i(r, u) \sigma_n(u') = \phi_i(r, u) \sigma_n(u) - (u - u') \frac{\partial}{\partial u} [\phi_i(r, u) \sigma_n(u)] + \dots$$

Considering, for the moment, only the isotropic case, we have on substituting (1.8) into (1.4)

$$Q_n(r, u) = \int_0^u \left\{ \phi_o(r, u) \sigma_n(u) - (u - u') \frac{\partial}{\partial u} [\phi_o(r, u) \sigma_n(u)] \right\} \int_u^\infty J_n(u' \rightarrow u'') du'' du' \quad (1.9)$$

or

$$Q_n(r, u) = \int_0^u \left\{ \phi_o(r, u) \sigma_n(u) - (u - u') \frac{\partial}{\partial u} [\phi_o(r, u) \sigma_n(u)] \right\} \int_u^\infty \frac{e^{u' - u''}}{1 - \alpha} du'' du'$$

Performing the u'' integration yields

$$Q_n(r, u) = \phi_o(r, u) \sigma_n(u) \int_0^u \left\{ \frac{e^{u' - u}}{1 - \alpha} - \frac{\alpha}{1 - \alpha} \right\} + \frac{\partial}{\partial u} [\phi_o(r, u) \sigma_n(u)] \int_0^u (u' - u) \left\{ \frac{e^{u' - u}}{1 - \alpha} - \frac{\alpha}{1 - \alpha} \right\} du'$$

Integrating again

$$Q_n(r, u) = \xi_n \phi_o(r, u) \sigma_n(u) + \frac{\partial}{\partial u} [\phi_o(r, u) \sigma_n(u)] \left[\xi_n + \frac{a_n \ln^2 a_n}{2(1 - a_n)} \right] \quad (1.10)$$

where $\xi_n = 1 + \frac{a_n \ln a_n}{1 - a_n}$

which is the average logarithmic energy loss per collision. If we let

$$a_n = \frac{a_n \ln^2 a_n}{1 - a_n} - \xi_n$$

then (1.10) may be written as

$$Q_n(r, u) = \xi_n \phi_o(r, u) \sigma_n(u) + a_n \frac{\partial}{\partial u} [\phi_o(r, u) \sigma_n(u)] \quad (1.11)$$

If the expansion of the collision density is now substituted into (1.6)

noting that

$$\int_0^u (u-u') J_n(u' \rightarrow u) du' = \frac{1}{1-\alpha_n} \int_{u+\ln \alpha_n}^u (u-u') e^{u'-u} du' = \xi_n^{(3)} \quad (3)$$

we see that

$$\frac{\partial}{\partial u} [\phi_0(r, u) \sigma_n(u)] = \frac{1}{\xi_n} \frac{\partial Q_n(r, u)}{\partial u} \quad (1.12)$$

Equation (1.11) now takes the form

$$Q_n(r, u) = \xi_n \phi_0(r, u) \sigma_n(u) + \frac{Q_n}{\xi_n} \frac{\partial Q_n(r, u)}{\partial u}$$

or

$$\gamma_n \frac{\partial Q_n(r, u)}{\partial u} + Q_n(r, u) = \xi_n \phi_0(r, u) \sigma_n(u) \quad (1.13)$$

with

$$\gamma_n = -\frac{Q_n}{\xi_n}$$

Equation (1.13) is part of the result we were seeking; that is, the

evaluation of the isotropic scattering integral in terms of $Q_n(r, u)$.

The P_1 slowing down density will now be treated in an analogous manner. As before, if we substitute the appropriate expression from (1.8) into equation (1.5) we get

$$P_n(r, u) = \int_0^u \left\{ \phi_1(r, u) \sigma_n(u) - (u-u') \frac{\partial}{\partial u} [\phi_1(r, u) \sigma_n(u)] \right\} \int_u^\infty K_n(u' \rightarrow u'') du'' du' \quad (1.14)$$

Substituting in the value of $K_n(u' \rightarrow u)$ we get

$$P_n(r, u) = \int_0^u \left\{ \phi_1(r, u) \sigma_n(u) - (u-u') \frac{\partial}{\partial u} [\phi_1(r, u) \sigma_n(u)] \right\} \frac{1}{2(1-\alpha_n)} \int_u^{u'-\ln \alpha_n} \left[(A_n+1) e^{\frac{3}{2}(u'-u'')} - (A_n-1) e^{\frac{1}{2}(u'-u'')} \right] du''$$

Integrating over u'' yields

$$P_n(r, u) = \frac{A_n+1}{2(\alpha_n-1)} \phi_1(r, u) \sigma_n(u) \int_{u+\ln \alpha_n}^u \left\{ 2\alpha_n \left(\frac{\alpha_n^{\frac{1}{2}}}{3} - 1 \right) - \frac{2}{3} e^{\frac{3}{2}(u'-u)} + 2\alpha_n^{\frac{1}{2}} e^{\frac{1}{2}(u'-u)} \right\} du' \\ + \frac{A_n+1}{2(\alpha_n-1)} \frac{\partial}{\partial u} [\phi_1(r, u) \sigma_n(u)] \int_{u+\ln \alpha_n}^u (u'-u) \left\{ 2\alpha_n \left(\frac{\alpha_n^{\frac{1}{2}}}{3} - 1 \right) - \frac{2}{3} e^{\frac{3}{2}(u'-u)} + 2\alpha_n^{\frac{1}{2}} e^{\frac{1}{2}(u'-u)} \right\} du' \quad (1.15)$$

(3) See Appendix

Integrating again

$$P_n(r, u) = \frac{A_n+1}{2(A_n-1)} \phi_1(r, u) \sigma_n(u) \left\{ -2q_n \ln q_n \left(\frac{q_n^{\frac{1}{3}}}{3} - 1 \right) - \frac{4}{9} (1 - q_n^{\frac{2}{3}}) + 4q_n^{\frac{1}{3}} (1 - q_n^{\frac{1}{3}}) \right\} \\ + \frac{A_n+1}{2(A_n-1)} \frac{\partial}{\partial u} \phi_1(r, u) \sigma_n(u) \left\{ -q_n \ln^2 q_n \left(\frac{q_n^{\frac{1}{3}}}{3} - 1 \right) - \frac{4}{9} \left[\frac{2}{3} (q_n^{\frac{1}{3}} - 1) - q_n^{\frac{2}{3}} \ln q_n \right] + 4q_n^{\frac{1}{3}} \left[2(q_n^{\frac{1}{3}} - 1) - q_n^{\frac{1}{3}} \ln q_n \right] \right\} \quad (1.16)$$

If we denote the coefficient of $\phi_1(r, u) \sigma_n(u)$ by η_n and the coefficient of $\frac{\partial}{\partial u} [\phi_1(r, u) \sigma_n(u)]$ by b_n then, similarly to before, we have

$$P_n(r, u) = \eta_n \phi_1(r, u) \sigma_n(u) - b_n \frac{\partial}{\partial u} [\phi_1(r, u) \sigma_n(u)] \quad (1.17)$$

Substituting (1.8) into equation (1.7), noting that

$$\int_0^u (u-u') K_n(u' \rightarrow u) du' = \frac{1}{2(1-q_n)} \int_0^u \left\{ (u'-u) \left[(A_n+1) e^{\frac{2}{3}(u'-u)} - (A_n-1) e^{\frac{1}{3}(u'-u)} \right] \right\} du' = \eta_n$$

leads to the result

$$\frac{\partial}{\partial u} [\phi_1(r, u) \sigma_n(u)] = \frac{1}{\eta_n} \frac{\partial P_n(r, u)}{\partial u}$$

Introducing this into equation (1.17) we get

or

$$\rho_n \frac{\partial P_n(r, u)}{\partial u} + P_n(r, u) = \eta_n \phi_1(r, u) \sigma_n(u) \quad (1.18)$$

with

$$\rho_n = \frac{b_n}{\eta_n}$$

Equation (1.18) together with equation (1.13) constitute the result we have been seeking; that is, the evaluation of the scattering integrals in terms of $Q_n(r, u)$ and $P_n(r, u)$.

For completeness, we will now write equations (1.1) and (1.2) in terms of $Q_n(r, u)$ and $P_n(r, u)$. This is accomplished by substituting (1.7) into (1.1) and (1.6) into (1.2). The resulting expressions are

(4) See Appendix

$$\frac{1}{3} \nabla_0 \phi_0(r, u) + \sum_n \{ \tau_n(u) - \bar{\mu}_n \sigma_n(u) \} \phi_1(r, u) + \sum_n \frac{\partial}{\partial u} P_n(r, u) = 0 \quad (1.19)$$

$$\nabla_1 \phi_1(r, u) = S(r, u) - \sum_n \alpha_n(u) \phi_0(r, u) - \sum_n \frac{\partial}{\partial u} Q_n(r, u) \quad (1.20)$$

where $\alpha_n(u) = \tau_n(u) - \sigma_n(u)$

Thus a set of partial differential equations describing the consistent P_1 approximation to the Boltzmann equation have been obtained. For the sake of convenience, they are tabulated below:

$$\gamma_n \frac{\partial Q_n(r, u)}{\partial u} + Q_n(r, u) = \sum_n \phi_0(r, u) \sigma_n(u) \quad (1.13)$$

$$P_n \frac{\partial P_n(r, u)}{\partial u} + P_n(r, u) = \gamma_n \phi_1(r, u) \sigma_n(u) \quad (1.18)$$

$$\frac{1}{3} \nabla_0 \phi_0(r, u) + \sum_n \{ \tau_n(u) - \bar{\mu}_n \sigma_n(u) \} \phi_1(r, u) + \sum_n \frac{\partial}{\partial u} P_n(r, u) = 0 \quad (1.19)$$

$$\nabla_1 \phi_1(r, u) = S(r, u) - \sum_n \alpha_n(u) \phi_0(r, u) - \sum_n \frac{\partial}{\partial u} Q_n(r, u) \quad (1.20)$$

II. CLASSES OF ELEMENTS

The P_1 differential equations obtained in Section I describing the slowing down densities represent first order approximations and are applicable to all classes of elements; i.e., for all values of mass number A. ⁽¹⁾ Since for many elements the solutions to these equations can be greatly simplified, we will introduce three classes of elements and the form of the slowingdown which must be satisfied.

We will consider first a class A such that

$$\frac{\partial Q_n(r,u)}{\partial u} = -\alpha_n(u) \phi_0(r,u) \quad (2.1)$$

$$\frac{\partial P_n(r,u)}{\partial u} = -\beta_n(u) \phi_1(r,u) \quad (2.2)$$

where

$$\alpha_n(u) = \tau_n(u) - \sigma_n(u)$$

$$\beta_n(u) = \alpha_n(u) + \sigma_n(1 - \bar{\tau}_{on})$$

If we substitute equation (2.1) into (1.13) the resulting expression is

$$Q_n(r,u) = \left\{ \tau_n \sigma_n(u) + \sigma_n \alpha_n(u) \right\} \phi_0(r,u) \quad (2.3)$$

Similarly, substituting (2.2) into (1.18)

$$P_n(r,u) = \left\{ \tau_n \sigma_n(u) + \rho_n \alpha_n(u) \right\} \phi_1(r,u) \quad (2.4)$$

⁽¹⁾ This, of course, is assuming that the expansions utilized in Section I are valid.

For class B we will allow the above to be true for $P_n(x,u)$ only.

Class C elements will naturally assume the general expressions; that is, equations (1.13) and (1.18).

In summary, we will categorize the elements in the following manner:

Class A

$$Q_n(x,u) = \left\{ \sum_n \sigma_n(u) + \gamma_n a_n(u) \right\} \phi_0(x,u) \quad (2.5)$$

$$P_n(x,u) = \left\{ \eta_n \sigma_n(u) + \rho_n a_n(u) \right\} \phi_1(x,u) \quad (2.6)$$

Class B

$$\gamma_n \frac{\partial}{\partial u} Q_n(x,u) + Q_n(x,u) = \sum_n \sigma_n(u) \phi_0(x,u) \quad (2.7)$$

$$P_n(x,u) = \left\{ \eta_n \sigma_n(u) + \rho_n a_n(u) \right\} \phi_1(x,u) \quad (2.8)$$

Class C

$$\gamma_n \frac{\partial}{\partial u} Q_n(x,u) + Q_n(x,u) = \sum_n \sigma_n(u) \phi_0(x,u) \quad (2.9)$$

$$\rho_n \frac{\partial}{\partial u} P_n(x,u) + P_n(x,u) = \eta_n \sigma_n(u) \phi_1(x,u) \quad (2.10)$$

These relations will be used in the following section to develop the group equations.

III. DEVELOPMENT OF THE GROUP EQUATIONS

A. Basic Assumption

In this section we will concern ourselves with the development of the group equations. In particular, we will perform the lethargy integration on the basic P_1 differential equations from Section I. It should be pointed out that the thermal group will not be included since it requires special attention. Therefore, it and the spatial integration will be treated in the two succeeding sections.

Utilizing equations (2.5) through (2.10) in equations (1.19) and (1.20) while reducing and rearranging leads to

$$\begin{aligned} \frac{1}{3} \nabla_0 \phi_0(r, u) + \sum_{AB} \left\{ \tau_n(u) - \bar{\mu}_n \sigma_n(u) + \eta_n \dot{\sigma}_n(u) + \rho_n \dot{\alpha}_n(u) \right\} \phi_i(r, u) \\ + \sum_c \left\{ \tau_n(u) - \bar{\mu}_n \sigma_n(u) + \frac{\eta_n}{\rho_n} \sigma_n(u) \right\} \phi_i(r, u) + \sum_{AB} \left\{ \eta_n \sigma_n(u) + \rho_n \dot{\alpha}_n(u) \right\} \dot{\phi}_i(r, u) \quad (3.1) \\ - \sum_c \frac{1}{\rho_n} \rho_n(r, u) = 0 \end{aligned}$$

$$\begin{aligned} \nabla_i \phi_i(r, u) = S(r, u) - \sum_A \left\{ \alpha_n(u) + \xi_n \dot{\sigma}_n(u) + \gamma_n \dot{\alpha}_n(u) \right\} \phi_0(r, u) \\ - \sum_A \left\{ \xi_n \sigma_n(u) + \gamma_n \alpha_n(u) \right\} \dot{\phi}_0(r, u) - \sum_{BC} \left\{ \alpha_n(u) + \frac{\xi_n}{\gamma_n} \sigma_n(u) \right\} \phi_0(r, u) \quad (3.2) \\ + \sum_{BC} \gamma_n' \alpha_n(r, u) \end{aligned}$$

now define

$$\begin{aligned}
T_0(u) &= \sum_A \left\{ \alpha_n(u) + \int_n \dot{\sigma}_n(u) + \gamma_n \dot{\alpha}_n(u) \right\} \\
&\quad + \sum_{B,C} \left\{ \alpha_n(u) + \frac{\int_n}{\gamma_n} \sigma_n(u) \right\} \\
T_1(u) &= \sum_{AB} \left\{ \tau_n(u) - \bar{\mu}_n \sigma_n(u) + \eta_n \dot{\sigma}_n(u) + \rho_n \dot{\alpha}_n(u) \right\} \\
&\quad + \sum_C \left\{ \tau_n(u) - \bar{\mu}_n \sigma_n(u) + \frac{\eta_n}{\rho_n} \sigma_n(u) \right\}
\end{aligned} \tag{3.3}$$

$$V_0(u) = \sum_A \left\{ \int_n \sigma_n(u) + \gamma_n \alpha_n(u) \right\}$$

$$V_1(u) = \sum_{AB} \left\{ \eta_n \sigma_n(u) + \rho_n \alpha_n(u) \right\}$$

$$p_n(r,u) = \frac{1}{\rho_n} P_n(r,u)$$

$$g_n(r,u) = \frac{1}{\gamma_n} Q_n(r,u)$$

Using the latter two expressions of (3.3) together with (2.7), (2.9) and (2.10) leads to

$$\dot{p}_n(r,u) = \frac{1}{\rho_n} \dot{P}_n(r,u) \tag{3.4}$$

$$\dot{g}_n(r,u) = \frac{1}{\gamma_n} \dot{Q}_n(r,u) \tag{3.5}$$

For class C

$$\rho_n \dot{\phi}_n(x, u) + \rho_n(x, u) = \frac{\eta_n}{\rho_n} \sigma_n(u) \phi_n(x, u) \quad (3.6)$$

For classes B and C

$$\gamma_n \dot{\phi}_n(x, u) + \gamma_n(x, u) = \frac{\xi_n}{\gamma_n} \sigma_n(u) \phi_n(x, u) \quad (3.7)$$

where the dot above the symbol indicates the lethargy derivative.⁽¹⁾

The relationships (3.4) through (3.7) will be useful when the integration is made.

Equations (3.1) and (3.2) now take the form

$$\frac{1}{3} \nabla_0 \phi_0(x, u) + T_1(u) \phi_1(x, u) + V_1(u) \dot{\phi}_1(x, u) - \sum_C \rho_n(u) = 0 \quad (3.8)$$

$$\nabla_1 \phi_1(x, u) = S(x, u) - T_0(u) \phi_0(x, u) - V_0(u) \dot{\phi}_0(x, u) + \sum_{Bc} \gamma_n(x, u) \quad (3.9)$$

Before we can perform the lethargy integration on (3.8) and (3.9), we will have to make certain simplifying assumptions on the lethargy dependence of the flux. This assumption will be one of flux linearity over a group interval and is represented by

$$\phi(u) = \frac{u - u_p}{u_{p+1} - u_p} \phi(u_{p+1}) - \frac{u_p - u}{u_{p+1} - u_p} \phi(u_p)$$

The group constants will be expressed in terms of the lower endpoint and midpoint flux. Therefore,

$$\phi(u) = \frac{1}{u_p} \left\{ 2(u - u_p) \phi(u_p) + (u_{p+1} + u_p - 2u) \phi(u_{p+1}) \right\} \quad (3.10)$$

where

⁽¹⁾ This notation will be used throughout this section.

$U_p = u_{p+1} - u_p = \text{lethargy interval}$

$\bar{\phi}(u_p) = \frac{1}{2} \{ \phi(u_{p+1}) + \phi(u_p) \} = \text{average (or midpoint) flux}$

$u_p = \text{lower lethargy limit of group}$

$u_{p+1} = \text{upper lethargy limit of group}$

On the basis of the above assumption, we will evaluate forms of integrals expected when (3.8) and (3.9) are integrated.

Consider
$$\frac{1}{U_p} \int_{u_p}^{u_{p+1}} \sigma(u) \phi(u) du$$

$$\frac{1}{U_p} \int_{u_p}^{u_{p+1}} \sigma(u) \phi(u) du = \sigma^*(u_p) \bar{\phi}(u_p) + \sigma^+(u_p) \phi(u_p) \quad (3.11)$$

where

$$\sigma^*(u_p) = \frac{1}{U_p^2} \int_{u_p}^{u_{p+1}} 2(u - u_p) \sigma(u) du \quad (3.12)$$

$$\sigma^+(u_p) = \frac{1}{U_p^2} \int_{u_p}^{u_{p+1}} (u_{p+1} + u_p - 2u) \sigma(u) du \quad (3.13)$$

now

$$\sigma^*(u_p) = \frac{2}{U_p^2} \int_{u_p}^{u_{p+1}} u \sigma(u) du - \frac{2u_p}{U_p^2} \int_{u_p}^{u_{p+1}} \sigma(u) du = \frac{2}{U_p} \sigma^+(u_p) - \frac{2u_p}{U_p} \bar{\sigma}(u_p) \quad (3.14)$$

where

$$\sigma^+(u_p) = \frac{1}{U_p} \int_{u_p}^{u_{p+1}} u \sigma(u) du \quad (3.15)$$

$$\bar{\sigma}(u_p) = \frac{1}{U_p} \int_{u_p}^{u_{p+1}} \sigma(u) du \quad (3.16)$$

For $\sigma^*(u_p)$ we have

$$\sigma^*(u_p) = \frac{1}{U_p^2} \int_{u_p}^{u_{p+1}} (u_{p+1} + u_p - 2u) \sigma(u) du = \bar{\sigma}(u_p) - \sigma^*(u_p) \quad (3.17)$$

Also consider $\frac{1}{U_p} \int_{u_p}^{u_{p+1}} \sigma(u) \dot{\phi}(u) du$

$$\frac{1}{U_p} \int_{u_p}^{u_{p+1}} \sigma(u) \dot{\phi}(u) du = \frac{2\bar{\sigma}(u_p)}{U_p} \{ \bar{\phi}(u_p) - \phi(u_p) \} \quad (3.18)$$

where $\bar{\phi}(u_p)$ and $\bar{\sigma}(u_p)$ have been defined previously.

Other relationships which will be useful are

$$\dot{\sigma}_n^+(u_p) = \frac{1}{U_p} \int_{u_p}^{u_{p+1}} u \dot{\sigma}_n(u) du = \frac{1}{U_p} \{ u_{p+1} \sigma_n(u_{p+1}) - u_p \sigma_n(u_p) \} - \bar{\sigma}_n(u_p) \quad (3.19)$$

$$\sigma^*(u_p) = \frac{u_{p+1} + u_p}{U_p} \bar{\sigma}(u_p) - \frac{2}{U_p} \sigma^+(u_p) \quad (3.20)$$

$$u_p \dot{\bar{\sigma}}(u_p) = \frac{u_p}{U_p} \{ \sigma_n(u_{p+1}) - \sigma_n(u_p) \} \quad (3.21)$$

$$*\dot{\sigma}(u_p) = \frac{2}{U_p} \{ \sigma_n(u_{p+1}) - \bar{\sigma}_n(u_p) \} \quad (3.22)$$

B. Integration

Making use of the relations developed in A while dividing through by U_p , equation (3.8) is integrated from u_p to u_{p+1} . The resulting expression is

$$\begin{aligned} & \frac{1}{3} \nabla_0 \bar{\phi}_0(x, u_p) + \tau_1^*(u_p) \bar{\phi}_1(x, u_p) + \tau_1^*(u_p) \phi_1(x, u_p) \\ & + \frac{2}{U_p} \{ \bar{\phi}_1(x, u_p) - \phi_1(x, u_p) \} \bar{V}_1(u_p) - \sum_c \bar{\phi}_n(u_p) = 0 \end{aligned} \quad (3.23)$$

Doing the same to equation (3.6) yields

$$\rho_n \frac{2}{U_p} \left\{ \bar{p}_n(z, u_p) - p_n(z, u_p) \right\} + \bar{p}_n(z, u_p) = \frac{\eta_n}{\rho_n} \left\{ \sigma_n^*(u_p) \bar{\phi}_1(z, u_p) + \sigma_n^*(u_p) \phi_1(z, u_p) \right\}$$

or

$$\bar{p}_n(z, u_p) = \frac{2\rho_n}{2\rho_n + U_p} p_n(z, u_p) + \frac{\eta_n U_p}{\rho_n(2\rho_n + U_p)} \left\{ \sigma_n^*(u_p) \bar{\phi}_1(z, u_p) + \sigma_n^*(u_p) \phi_1(z, u_p) \right\} \quad (3.24)$$

Substituting (3.24) into (3.23) we have

$$\begin{aligned} \frac{1}{3} \nabla_0 \bar{\phi}_0(z, u_p) + \left\{ T_1^*(u_p) + \frac{2\bar{V}_1(u_p)}{U_p} - \sum \frac{\eta_n}{\rho_n} \frac{U_p}{2\rho_n + U_p} \sigma_n^*(u_p) \right\} \bar{\phi}_1(z, u_p) \\ + \left\{ T_1^*(u_p) - \frac{2}{U_p} \bar{V}_1(u_p) - \sum \frac{\eta_n}{\rho_n} \frac{U_p}{2\rho_n + U_p} \sigma_n^*(u_p) \right\} \phi_1(z, u_p) - \sum \frac{2\rho_n}{2\rho_n + U_p} p_n(z, u_p) = 0 \end{aligned} \quad (3.25)$$

Now if we perform a similar integration on equation (3.9), we get

$$\begin{aligned} \nabla_1 \bar{\phi}_1(z, u_p) = \bar{S}(z, u_p) - T_0^*(u_p) \bar{\phi}_0(z, u_p) - T_0^*(u_p) \phi_0(z, u_p) \\ - \frac{2}{U_p} \left\{ \bar{\phi}_0(z, u_p) - \phi_0(z, u_p) \right\} \bar{V}_0(u_p) + \sum_{8c} \bar{g}_n(z, u_p) \end{aligned} \quad (3.26)$$

As before, integrating (3.7) while dividing by U_p leads to

$$\bar{g}_n(z, u_p) = \frac{2\delta_n}{2\delta_n + U_p} g_n(z, u_p) + \frac{\xi_n}{\delta_n} \frac{U_p}{2\delta_n + U_p} \left\{ \sigma_n^*(u_p) \bar{\phi}_0(z, u_p) + \sigma_n^*(u_p) \phi_0(z, u_p) \right\} \quad (3.27)$$

Substituting into (3.26)

$$\begin{aligned} \nabla_1 \bar{\phi}_1(z, u_p) = \bar{S}(z, u_p) - \bar{\phi}_0(z, u_p) \left\{ T_0^*(u_p) + \frac{2}{U_p} \bar{V}_0(u_p) - \sum_{8c} \frac{\xi_n}{\delta_n} \frac{U_p}{2\delta_n + U_p} \sigma_n^*(u_p) \right\} \\ - \left\{ T_0^*(u_p) - \frac{2}{U_p} \bar{V}_0(u_p) - \sum_{8c} \frac{\xi_n}{\delta_n} \frac{U_p}{2\delta_n + U_p} \sigma_n^*(u_p) \right\} \phi_0(z, u_p) + \sum_{8c} \frac{2\delta_n}{2\delta_n + U_p} g_n(z, u_p) \end{aligned} \quad (3.28)$$

Considering equations (3.25) and (3.28), we now define

$$\begin{aligned}
 A(u_p) &= 3 \left\{ T_1^*(u_p) + \frac{2 \bar{V}_1(u_p)}{U_p} - \sum_{BC} \frac{\eta_n}{\rho_n} \frac{U_p}{2 \rho_n + U_p} T_n^*(u_p) \right\} \\
 B(x, u_p) &= 3 \left\{ T_1^*(u_p) - \frac{2 \bar{V}_1(u_p)}{U_p} - \sum_{BC} \frac{\eta_n}{\rho_n} \frac{U_p}{2 \rho_n + U_p} T_n^*(u_p) \right\} \phi_1(x, u_p) - 3 \sum_{BC} \frac{2 \rho_n}{2 \rho_n + U_p} \phi_n(x, u_p) \\
 C(u_p) &= T_0^*(u_p) + \frac{2 \bar{V}_0(u_p)}{U_p} - \sum_{BC} \frac{\xi_n}{\delta_n} \frac{U_p}{2 \delta_n + U_p} T_n^*(u_p) \\
 D(x, u_p) &= \bar{S}(x, u_p) - \left\{ T_0^*(u_p) - \frac{2 \bar{V}_0(u_p)}{U_p} - \sum_{BC} \frac{\xi_n}{\delta_n} \frac{U_p}{2 \delta_n + U_p} T_n^*(u_p) \right\} \phi_0(x, u_p) + \sum_{BC} \frac{2 \delta_n}{2 \delta_n + U_p} \phi_n(x, u_p)
 \end{aligned} \tag{3.29}$$

Rewriting (3.25) and (3.28)

$$\nabla_0 \bar{\phi}_0(x, u_p) + A(u_p) \bar{\phi}_1(x, u_p) + B(x, u_p) = 0 \tag{3.30}$$

$$\nabla_1 \bar{\phi}_1(x, u_p) = -C(u_p) \bar{\phi}_0(x, u_p) + D(x, u_p) \tag{3.31}$$

It is now convenient to reduce these equations to a single equation.

To do this, operate on (3.30) with ∇_1 . This results in

$$\nabla_1 \nabla_0 \bar{\phi}_0(x, u_p) + \nabla_1 A(u_p) \bar{\phi}_1(x, u_p) + \nabla_1 B(x, u_p) = 0$$

Substituting from (3.31) gives

$$\nabla^2 \bar{\phi}_0(x, u_p) + A(u_p) \{ -C(u_p) \bar{\phi}_0(x, u_p) + D(x, u_p) \} + \nabla_1 B(x, u_p) = 0$$

Expanding

$$\nabla^2 \bar{\phi}_0(x, u_p) - A(u_p) C(u_p) \bar{\phi}_0(x, u_p) + A(u_p) D(x, u_p) + \nabla_1 B(x, u_p) = 0 \tag{3.32}$$

Note that

$$\bar{\phi}_1(x, u_p) = -\frac{1}{A(u_p)} \{ \nabla_0 \bar{\phi}_0(x, u_p) + B(x, u_p) \} \tag{3.33}$$

C. Group Constants

Here we will attempt to evaluate the group coefficients (as defined by (3.29) in terms of known quantities. We will begin by examining $A(u_p)$.

If we rewrite $A(u_p)$ making use of equation (3.14) we get

$$A(u_p) = 3 \left\{ \frac{2}{U_p} T_1^+(u_p) - \frac{2u_p}{U_p} \bar{T}_1(u_p) + \frac{2}{U_p} \bar{V}_1(u_p) \right. \\ \left. - \sum_c \frac{\eta_n}{\rho_n} \frac{U_p}{2\rho_n + U_p} \left\{ \frac{2}{U_p} \sigma_n^+(u_p) - \frac{2u_p}{U_p} \bar{\sigma}_n(u_p) \right\} \right\} \quad (3.34)$$

It is observed that we still have need to evaluate $\bar{T}_1(u_p)$, $T_1^+(u_p)$

and $\bar{V}_1(u_p)$. Therefore, from (3.3) together with (3.15) and (3.16), we have

$$\bar{T}_1(u_p) = \frac{1}{U_p} \int_{u_p}^{u_{p+1}} T_1(u) du = \sum_{AB} \left\{ \bar{\tau}_n(u_p) - \bar{\mu}_{on} \bar{\sigma}_n(u_p) + \frac{\eta_n}{U_p} [\sigma_n(u_{p+1}) - \sigma_n(u_p)] \right. \quad (3.35)$$

$$\left. + \frac{\rho_n}{U_p} [\alpha_n(u_{p+1}) - \alpha_n(u_p)] \right\} + \sum_c \left\{ \bar{\tau}_n(u_p) + \left(\frac{\eta_n}{\rho_n} - \bar{\mu}_{on} \right) \bar{\sigma}_n(u_p) \right\}$$

$$T_1^+(u_p) = \frac{1}{U_p} \int_{u_p}^{u_{p+1}} u T_1(u) du = \sum_{AB} \left\{ \tau_n^+(u_p) - \bar{\mu}_{on} \sigma_n^+(u_p) + \frac{\eta_n}{U_p} [u_{p+1} \sigma_n(u_{p+1}) - u_p \sigma_n(u_p)] \right. \\ \left. - \eta_n \bar{\sigma}_n(u_p) + \frac{\rho_n}{U_p} [u_{p+1} \alpha_n(u_{p+1}) - u_p \alpha_n(u_p)] - \rho_n \bar{\alpha}_n(u_p) \right\} \quad (3.36)$$

$$+ \sum_c \left\{ \tau_n^+(u_p) + \left(\frac{\eta_n}{\rho_n} - \bar{\mu}_{on} \right) \sigma_n^+(u_p) \right\}$$

$$\bar{V}_1(u_p) = \frac{1}{U_p} \int_{u_p}^{u_{p+1}} V_1(u) du = \\ = \sum_{AB} \left\{ \eta_n \bar{\sigma}_n(u_p) + \rho_n \bar{\alpha}_n(u_p) \right\} \quad (3.37)$$

Substituting into equation (3.34) and reducing leads to

$$\begin{aligned}
 A(u_p) = & \frac{1}{U_p} \left(\sum_{ABC} \left\{ \tau_n^+(u_p) - u_p \bar{\tau}_n(u_p) \right\} \right. \\
 & - \sum_{AB} \left[\bar{\mu}_n \left\{ \sigma_n^+(u_p) - u_p \bar{\sigma}_n(u_p) \right\} - \gamma_n \sigma_n(u_{p+1}) - \rho_n \alpha_n(u_{p+1}) \right] \\
 & \left. + \sum_C \left\{ \frac{\gamma_n}{\rho_n} \frac{2\rho_n}{2\rho_n + U_p} - \bar{\mu}_n \right\} \left\{ \sigma_n^+(u_p) - u_p \bar{\sigma}_n(u_p) \right\} \right)
 \end{aligned} \quad (3.38)$$

Considering from (3.29) $C(u_p)$, we again make use of (3.14) and rearrange.

The resulting expression is

$$\begin{aligned}
 C(u_p) = & \frac{2}{U_p} T_o^+(u_p) - \frac{2u_p}{U_p} \bar{T}_o(u_p) + \frac{2}{U_p} \bar{V}_o(u_p) \\
 & - \sum_{BC} \frac{\xi_n}{\gamma_n} \frac{U_p}{2\gamma_n + U_p} \left\{ \frac{2}{U_p} \sigma_n^+(u_p) - \frac{2u_p}{U_p} \bar{\sigma}_n(u_p) \right\}
 \end{aligned} \quad (3.39)$$

In this case we have to evaluate $\bar{T}_o(u_p)$, $T_o^+(u_p)$ and $\bar{V}_o(u_p)$

Therefore, as for $A(u_p)$ we utilize equations (3.3), (3.15) and (3.16).

$$\begin{aligned}
 \bar{T}_o(u_p) = & \frac{1}{U_p} \int_{u_p}^{u_{p+1}} \bar{T}_o(u) du = \sum_A \left\{ \bar{\alpha}_n(u_p) + \xi_n \left[\frac{\sigma_n(u_{p+1}) - \sigma_n(u_p)}{U_p} \right] \right. \\
 & \left. + \gamma_n \left[\frac{\alpha_n(u_{p+1}) - \alpha_n(u_p)}{U_p} \right] \right\} \\
 & + \sum_{BC} \left\{ \bar{\alpha}_n(u_p) + \frac{\xi_n}{\gamma_n} \bar{\sigma}_n(u_p) \right\}
 \end{aligned} \quad (3.40)$$

$$\begin{aligned}
 T_o^+(u_p) = & \frac{1}{U_p} \int_{u_p}^{u_{p+1}} u T_o(u) du = \sum_A \left\{ \alpha_n^+(u_p) + \xi_n \dot{\sigma}_n^+(u_p) + \gamma_n \dot{\alpha}_n^+(u_p) \right\} \\
 & + \sum_{BC} \left\{ \alpha_n^+(u_p) + \frac{\xi_n}{\gamma_n} \sigma_n^+(u_p) \right\}
 \end{aligned} \quad (3.41)$$

$$\begin{aligned}
 \bar{V}_o(u_p) = & \frac{1}{U_p} \int_{u_p}^{u_{p+1}} \bar{V}_o(u) du \\
 = & \sum_A \left\{ \xi_n \bar{\sigma}_n(u_p) + \gamma_n \bar{\alpha}_n(u_p) \right\}
 \end{aligned} \quad (3.42)$$

Substituting into (3.39) and rearranging gives

$$C(u_p) = \frac{2}{U_p} \left(\sum_{ABC} \left\{ \alpha_n^+(u_p) - u_p \bar{\alpha}_n(u_p) \right\} + \sum_A \left\{ \gamma_n \sigma_n(u_{p+1}) + \gamma_n \alpha_n(u_{p+1}) \right\} \right. \\ \left. + \sum_{BC} \left\{ \sigma_n^+(u_p) - u_p \bar{\sigma}_n(u_p) \right\} \frac{2 \xi_n}{2 \gamma_n + U_p} \right) \quad (3.43)$$

Looking at $B(x, u_p)$ we have on substituting (3.17) into the appropriate expression from (3.29)

$$B(x, u_p) = 3 \left\{ \bar{T}_1(u_p) - T_1(u_p) - \frac{2 \bar{V}_1(u_p)}{U_p} \right. \\ \left. - \sum_c \frac{\gamma_n}{\rho_n} \frac{U_p}{2 \rho_n + U_p} [\sigma_n(u_p) - \sigma_n^*(u_p)] \right\} \phi_1(x, u_p) - 3 \sum_c \frac{2 \rho_n}{2 \rho_n + U_p} \phi_n(x, u_p) \quad (3.44)$$

Rearranging, noting the expression for $A(u_p)$, yields

$$B(x, u_p) = \left\{ 3 \left[\bar{T}_1(u_p) - \sum_c \frac{\gamma_n}{\rho_n} \frac{U_p}{2 \rho_n + U_p} \bar{\sigma}_n(u_p) \right] - A(u_p) \right\} \phi_1(x, u_p) \\ - 3 \sum_c \frac{2 \rho_n}{2 \rho_n + U_p} \phi_n(x, u_p) \quad (3.45)$$

Using (3.35), together with equations (3.19) through (3.22), we have after reducing and arranging

$$B(x, u_p) = \left[3 \left(\sum_{ABC} \bar{\epsilon}_n(u_p) + \sum_{AB} \left\{ \frac{\gamma_n}{U_p} [\sigma_n(u_{p+1}) - \sigma_n(u_p)] \right. \right. \right. \\ \left. \left. - \bar{\mu}_n \bar{\sigma}_n(u_p) + \frac{2}{U_p} [\alpha_n(u_{p+1}) - \alpha_n(u_p)] \right\} \right) \right. \\ \left. + \sum_c \left(\frac{2 \gamma_n}{2 \rho_n + U_p} - \bar{\mu}_n \right) \bar{\sigma}_n(u_p) - A(u_p) \right] \phi_1(x, u_p) \quad (3.46)$$

Finally, for $D(x, u_p)$ we substitute the form of equation (3.17) into (3.29) getting

$$D(x, u_p) = \bar{S}(x, u_p) - \left\{ \bar{T}_2(u_p) - T_2(u_p) - \frac{2}{U_p} \bar{V}_2(u_p) \right. \\ \left. - \sum_{BC} \frac{\xi_n}{\gamma_n} \frac{U_p}{2 \gamma_n + U_p} [\bar{\sigma}_n(u_p) - \sigma_n^*(u_p)] \right\} \phi_0(x, u_p) + \sum_{BC} \frac{2 \gamma_n}{2 \gamma_n + U_p} \phi_n(x, u_p) \quad (3.47)$$

Rearranging, noting the value of $C(u_p)$ gives

$$D(x, u_p) = \bar{S}(x, u_p) - \left\{ -C(u_p) + \bar{T}_2(u_p) - \sum_{BC} \frac{\xi_n}{\gamma_n} \frac{U_p}{2 \gamma_n + U_p} \bar{\sigma}_n(u_p) \right\} \phi_0(x, u_p) \\ + \sum_{BC} \frac{2 \gamma_n}{2 \gamma_n + U_p} \phi_n(x, u_p) \quad (3.48)$$

From equation (3.40) combined with equations (3.19) through (3.22) we are able to reduce (3.48) to

$$D(x, u_p) = \bar{S}(x, u_p) - \left\{ \sum_A \left[\bar{\alpha}_n(u_p) + \frac{\rho_n}{U_p} \frac{\sigma_n(u_{p+1}) - \sigma_n(u_p) + \gamma_n \alpha_n(u_{p+1}) - \alpha_n(u_p)}{U_p} \right] \right. \\ \left. + \sum_{BC} \left[\bar{\alpha}_n(u_p) + \frac{\rho_n}{\gamma_n} \bar{\sigma}_n(u_p) \right] - \sum_{BC} \frac{\rho_n}{\gamma_n} \frac{U_p}{2\gamma_n + U_p} \sigma_n(u_p) - C(u_p) \right\} \phi_0(x, u_p) \\ + \sum_{BC} \frac{2\gamma_n}{2\gamma_n + U_p} g_n(x, u_p) \quad (3.49)$$

D. Summary

Summarizing the results we have

$$\nabla^2 \bar{\phi}_0(x, u_p) + \nabla_1 B(x, u_p) - A(u_p) C(u_p) \bar{\phi}_0(x, u_p) + A(u_p) D(x, u_p) = 0 \quad (3.32)$$

where

$$A(u_p) = \frac{6}{U_p} \left(\sum_{ABC} \left\{ \tau_n^+(u_p) - u_p \bar{\tau}_n(u_p) \right\} \right. \\ \left. - \sum_{ABC} \left[\bar{\mu}_n \left\{ \sigma_n^+(u_p) - u_p \bar{\sigma}_n(u_p) \right\} - \gamma_n \sigma_n(u_{p+1}) - \rho_n \bar{\alpha}_n(u_{p+1}) \right] \right. \\ \left. + \sum_C \left\{ \frac{\gamma_n}{\rho_n} \frac{2\rho_n}{2\rho_n + U_p} - \bar{\mu}_n \right\} \left\{ \sigma_n^+(u_p) - u_p \bar{\sigma}_n(u_p) \right\} \right) \quad (3.38)$$

$$B(x, u_p) = \left[3 \left(\sum_{ABC} \bar{\tau}_n(u_p) + \sum_{AB} \left\{ \frac{\gamma_n}{U_p} [\sigma_n'(u_{p+1}) - \sigma_n(u_p)] \right. \right. \right. \\ \left. \left. - \bar{\mu}_n \bar{\sigma}_n(u_p) + \frac{\rho_n}{U_p} [\alpha_n(u_{p+1}) - \alpha_n(u_p)] \right\} \right) \\ \left. + \sum_C \left(\frac{2\gamma_n}{2\rho_n + U_p} - \bar{\mu}_n \right) \bar{\sigma}_n(u_p) - A(u_p) \right] \phi_1(x, u_p) \quad (3.46)$$

$$C(u_p) = \frac{2}{U_p} \left(\sum_{ABC} \left\{ \alpha_n^+(u_p) - u_p \bar{\alpha}_n(u_p) \right\} + \sum_A \left\{ \rho_n \sigma_n(u_{p+1}) + \gamma_n \alpha_n(u_{p+1}) \right\} \right. \\ \left. + \sum_{BC} \left\{ \sigma_n^+(u_p) - u_p \bar{\sigma}_n(u_p) \right\} \frac{2\gamma_n}{2\gamma_n + U_p} \right) \quad (3.43)$$

$$\begin{aligned}
D(x, u_p) = & \bar{S}(x, u_p) - \left\{ \sum_A [\bar{\alpha}_n(u_p) + \sum_n \frac{\sigma_n(u_{p+1}) - \sigma_n(u_p)}{u_p} + \delta_n \cdot \frac{\alpha_n(u_{p+1}) - \alpha_n(u_p)}{u_p}] \right. \\
& + \sum_{BC} [\bar{\alpha}_n(u_p) + \frac{\xi_n}{\delta_n} \bar{\sigma}_n(u_p)] - \sum_{BC} \frac{\xi_n}{\delta_n} \frac{u_p}{2\delta_n + u_p} \sigma_n(u_p) - c(u_p) \left. \right\} \phi_0(x, u_p) \quad (3.49) \\
& + \sum_{BC} \frac{2\delta_n}{2\delta_n + u_p} g_n(x, u_p)
\end{aligned}$$

IV. THERMAL GROUP

In considering the thermal group, we will make the following assumptions on the scattering kernels

$$\left. \begin{aligned} K_n(v' \rightarrow v) &= 0 \\ J_n(v' \rightarrow v) &= \delta(v - v') \end{aligned} \right\} \quad (4.1)$$

$$\frac{1}{3} \nabla_0 \phi_0(r, E) + \Sigma(r) \phi_1(E, r) = \sum_n \rho_n^{th}(E) \quad (4.2)$$

$$\nabla_1 \phi_1(E, r) = S(E, r) - \phi_0(E, r) \sum_n \alpha_n(r) + \sum_n \phi_n^{th}(E) \quad (4.3)$$

Now, consider the reaction rate

R = reaction rate, events/sec

$R = \sigma v$

Assuming that the neutrons and moderator atoms follow a Maxwell-Boltzmann distribution of velocity, we have for the case of one neutron

$$R(\bar{v}, T_m) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left(\frac{m}{2\pi k T_n} \right)^{3/2} e^{-\frac{m u^2}{2 k T_n}} \left(\frac{M}{2\pi k T_m} \right)^{3/2} e^{-\frac{M z^2}{2 k T_m}} R(u-z, 0) du dz \quad (4.4)$$

where

k = Boltzmann's constant

m = neutron mass

u = neutron velocity

T_n = neutron temperature

M = moderator mass

T_m = moderator temperature

$\bar{v}$ = average neutron speed = $\frac{2}{\sqrt{\pi}} \left(\frac{2 k T_n}{m} \right)^{1/2}$

letting $u = u - z$

$$R(\bar{v}, T_m) = \left(\frac{m}{2\pi k T_n} \right)^{3/2} \left(\frac{M}{2\pi k T_m} \right)^{3/2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} R(u, 0) e^{-\frac{m u^2}{2 k T_n}} e^{-\frac{m}{k T_n} u \cdot z} e^{-\left(\frac{m}{2 k T_n} + \frac{M}{2 k T_m} \right) z^2} du dz \quad (4.6)$$

$$R(\bar{v}, T_M) = \left\{ \frac{m}{2\pi k(T_n + \frac{m}{M} T_M)} \right\}^{\frac{3}{2}} \int_{\underline{u}} e^{-\frac{m \underline{u}^2}{2k(T_n + \frac{m}{M} T_M)}} R(\underline{u}, 0) d\underline{u} \quad (4.7)$$

Defining an effective temperature:

$$T_{\text{eff}} = T_n + \frac{m}{M} T_M \quad (4.8)$$

$$R(\bar{v}, T_{\text{eff}}) = \left(\frac{m}{2\pi k T_{\text{eff}}} \right)^{\frac{3}{2}} \int_{\underline{u}} e^{-\frac{m \underline{u}^2}{2k T_{\text{eff}}}} R(|\underline{u}|, 0) d\underline{u}$$

so that

$$\sigma(\bar{v}, T_{\text{eff}}) = \left(\frac{m}{2\pi k T_{\text{eff}}} \right)^{\frac{3}{2}} \int_{\underline{u}} e^{-\frac{m \underline{u}^2}{2k T_{\text{eff}}}} \frac{|\underline{u}|}{\bar{v}} \sigma(|\underline{u}|, 0) d\underline{u} \quad (4.9)$$

Writing (4.2) and (4.3) in terms of average fluxes given

$$\frac{1}{3} \nabla_0 \bar{\phi}_0(r) + \bar{\phi}_1(r) \sum_n \bar{\tau}_n - \sum_n \rho_n^{\text{th}}(r) = 0 \quad (4.10)$$

$$\nabla_1 \bar{\phi}_1(r) = \bar{S}(r) - \bar{\phi}_0(r) \sum_n \bar{a}_n + \sum_n Q_n^{\text{th}}(r) \quad (4.11)$$

Operating on (4.10) with ∇_1 and substituting from (4.11)

$$\frac{1}{3} \nabla^2 \bar{\phi}_0(r) + \sum_n \bar{\tau}_n \left\{ \bar{S}(r) - \bar{\phi}_0(r) \sum_n \bar{a}_n + \sum_n Q_n^{\text{th}}(r) \right\} - \sum_n \rho_n^{\text{th}}(r) = 0 \quad (4.12)$$

$$\begin{aligned} \nabla^2 \bar{\phi}_0(r) - 3 \sum_n \bar{\tau}_n \sum_n \bar{a}_n \bar{\phi}_0(r) - \sum_n \bar{\tau}_n \bar{S}(r) \\ - \sum_n \bar{\tau}_n \sum_n Q_n^{\text{th}}(r) - \sum_n \rho_n^{\text{th}}(r) = 0 \end{aligned} \quad (4.13)$$

It is possible to go from one thermal group to another rather simply.

The Fermi Age expression for slowing down density is

$$Q(r, t) = \left(\frac{1}{4\pi t} \right)^{\frac{3}{2}} \int_{\underline{u}} e^{-\frac{\underline{u}^2}{4t}} Q(\underline{u}, 0) d\underline{u} \quad (4.14)$$

Identifying (4.8) with (4.14) shows

$$\bar{\tau} = \frac{k T_{\text{eff}}}{2 m v} \quad (4.15)$$

and R will satisfy the equation

$$\nabla_{\vec{r}}^2 R(\vec{r}, T_{eff}) = \frac{\partial}{\partial T} R(\vec{r}, T_{eff})$$

or

$$\frac{k}{2m} R''(\vec{r}, T_{eff}) = \frac{\partial}{\partial T_{eff}} R(\vec{r}, T_{eff}) \quad (4.16)$$

and boundary condition

$$R(\vec{r}, 0) = \delta(\vec{r})$$

Writing (4.17) in difference equation form:

$$\frac{R(\vec{r}, T_{eff} + l) - R(\vec{r}, T_{eff})}{l} = \frac{k}{2m} \frac{R(\vec{r} + h, T_{eff}) - 2R(\vec{r}, T_{eff}) + R(\vec{r} - h, T_{eff})}{h^2} \quad (4.17)$$

Consider the Fourier transform:

$$\psi(\omega, T) = \int_{-\infty}^{\infty} e^{i\omega x} R(x, T) dx \quad (4.18)$$

Expanding in powers of ω :

$$\psi(\omega, T) = \int_{-\infty}^{\infty} \left\{ 1 + i\omega x - \frac{\omega^2}{2!} x^2 + \dots \right\} R(x, T) dx \quad (4.19)$$

It is seen that the coefficients in the expansion are the moments.

Taking the Fourier transform of (4.17) yields

$$\frac{\psi(\omega, T+l) - \psi(\omega, T)}{l} = \frac{k}{2m} \frac{e^{-i\omega h} - 2 + e^{i\omega h}}{h^2} \psi(\omega, T) \quad (4.20)$$

$$\psi(\omega, T+l) = \left[1 - \frac{k}{im} \frac{l}{h^2} (1 - \cos \omega h) \right] \psi(\omega, T) \quad (4.21)$$

$$\psi(\omega, 0) = 1 \quad (4.22)$$

so

$$\psi(\omega, T) = \left[1 - \frac{k}{im} \frac{l}{h^2} (1 - \cos \omega h) \right]^{\frac{T}{l}} \quad (4.23)$$

The moments of the distribution

$$\left(\frac{m}{2\pi kT}\right)^{3/2} e^{-\frac{mv^2}{2kT}}$$

are

$$\left. \begin{aligned} M_0 &= 1 \\ M_1 &= M_3 = 0 \\ M_2 &= \frac{kT}{m} \\ M_4 &= 3 \frac{k^2 T^2}{m^2} \end{aligned} \right\} \quad (4.24)$$

Expanding $\psi(\omega, T)$ in (4.23)

$$1 - \cos \omega h = \frac{(\omega h)^2}{2!} - \frac{(\omega h)^4}{4!} + \dots \quad (4.25)$$

$$\psi(\omega, T) = 1 - \frac{\omega^2}{2!} \frac{k}{m} T + \frac{\omega^4}{4!} \left\{ \frac{T k h^2}{m} + \frac{T}{2} \left(\frac{T}{2} - 1 \right) \frac{1}{2!} \left(\frac{k}{m} \frac{l^2}{h^2} \right)^2 \frac{h^4}{4!} \right\} + \dots \quad (4.26)$$

and matching the fourth moment gives

$$l = \frac{h^2}{6} \frac{2m}{k} \quad (4.27)$$

so that (4.17) becomes

$$R(\bar{v}, T_{\text{eff}} + \frac{h^2}{3} \frac{m}{k}) = \frac{1}{6} \left\{ R(\bar{v} + h, T_{\text{eff}}) + 4 R(\bar{v}, T_{\text{eff}}) + R(\bar{v} - h, T_{\text{eff}}) \right\} \quad (4.28)$$

$$\sigma(\bar{v}, T_{\text{eff}} + \frac{h^2}{3} \frac{m}{k}) = \frac{1}{6\bar{v}} \left\{ (\bar{v} + h) \sigma(\bar{v} + h, T_{\text{eff}}) + 4\bar{v} \sigma(\bar{v}, T_{\text{eff}}) + (\bar{v} - h) \sigma(\bar{v} - h, T_{\text{eff}}) \right\} \quad (4.29)$$

V. SPATIAL INTEGRATION

A. Difference Equation

Equation (3.32) is

$$\bar{\Phi}_0''(z, u_p) + \frac{2}{h} \bar{\Phi}_0'(z, u_p) - \delta(u_p) \bar{\Phi}_0(z, u_p) + B'(z, u_p) + \frac{2}{h} B(z, u_p) + A(u_p) D(z, u_p) = 0 \quad (5.1)$$

where

$$\delta(u_p) = A(u_p) C(u_p) + B_g^2(u)$$

$$B_g^2(u) = \text{Geometric buckling}$$

The difference approximations are

$$\left. \begin{aligned} \psi''(r) &= \frac{\psi(r+h) - 2\psi(r) + \psi(r-h)}{h^2} \\ \psi'(r) &= \frac{\psi(r+h) - \psi(r-h)}{2h} \end{aligned} \right\} \quad (5.2)$$

If the right hand sides of (5.2) are expanded about r , there results

$$\left. \begin{aligned} \frac{\psi(r+h) - 2\psi(r) + \psi(r-h)}{h^2} &\sim \psi''(r) + \frac{h^2}{12} \psi''''(r) \\ \frac{\psi(r+h) - \psi(r-h)}{2h} &\sim \psi'(r) + \frac{h^2}{6} \psi'''(r) \end{aligned} \right\} \quad (5.3)$$

Approximations to the second and first derivatives, then, which are good to fourth order are

$$\left. \begin{aligned} \psi''(r) &= \frac{\psi(r+h) - 2\psi(r) + \psi(r-h)}{h^2} - \frac{h^2}{12} \psi''''(r) \\ \psi'(r) &= \frac{\psi(r+h) - \psi(r-h)}{2h} - \frac{h^2}{6} \psi'''(r) \end{aligned} \right\} \quad (5.4)$$

Substituting from (5.4) into (5.1) and understanding the equation applies to the p^{th} group gives

$$\begin{aligned} & \frac{\phi(r+h) - 2\phi(r) + \phi(r-h)}{h^2} + \frac{q}{r} \frac{\phi(r+h) - \phi(r-h)}{2h} - \delta \phi(r) \\ & - \frac{h^2}{12} \left\{ \phi^{(IV)}(r) + \frac{2q}{r} \phi'''(r) \right\} + \frac{B(r+h) - B(r-h)}{2h} + \frac{q}{r} B(r) \\ & - \frac{h^2}{6} B'''(r) + AD(r) = 0 \end{aligned} \quad (5.5)$$

Differentiating (5.1):

$$\phi'''(r) + \frac{q}{r} \phi''(r) - \frac{q}{r^2} \phi'(r) - \delta \phi'(r) + B''(r) + \frac{q}{r} B'(r) - \frac{q}{r^2} B(r) + AD'(r) = 0 \quad (5.6)$$

$$\phi'''(r) = - \left\{ \frac{q}{r} \phi''(r) - \left[\frac{q}{r^2} + \delta \right] \phi'(r) + B''(r) + \frac{q}{r} B'(r) - \frac{q}{r^2} B(r) + AD'(r) \right\} \quad (5.7)$$

Differentiating (5.6):

$$\begin{aligned} \phi^{(IV)}(r) + \frac{q}{r} \phi'''(r) = & - \left\{ - \frac{q}{r^2} \phi''(r) - \frac{q}{r^2} \phi''(r) + \frac{2q}{r^3} \phi'(r) - \delta \phi''(r) + B'''(r) \right. \\ & \left. + \frac{q}{r} B''(r) - \frac{q}{r^2} B'(r) - \frac{q}{r^2} B'(r) + \frac{2q}{r^3} B(r) + AD''(r) \right\} \end{aligned} \quad (5.8)$$

$$\begin{aligned} \phi^{(IV)}(r) + \frac{q}{r} \phi'''(r) = & - \left\{ \left[\frac{2q}{r^2} + \delta \right] \phi''(r) + \frac{2q}{r^3} \phi'(r) + B'''(r) + \frac{q}{r} B''(r) \right. \\ & \left. - \frac{2q}{r^2} B'(r) + \frac{2q}{r^3} B(r) + AD''(r) \right\} \end{aligned} \quad (5.9)$$

Multiplying (5.7) by $\frac{q}{r}$ and adding to (5.9):

$$\begin{aligned} \phi^{(IV)}(r) + \frac{2q}{r} \phi'''(r) = & - \left\{ \left(\frac{q^2}{r^2} - \frac{2q}{r^2} - \delta \right) \phi''(r) + \left[\frac{2q}{r^3} - \frac{q}{r} \left(\frac{q}{r^2} + \delta \right) \right] \phi'(r) \right. \\ & + B'''(r) + \frac{2q}{r} B''(r) + \left(\frac{q^2}{r^2} - \frac{2q}{r^2} \right) B'(r) \\ & \left. + \left(\frac{2q}{r^3} - \frac{q^2}{r^3} \right) B(r) + \frac{q}{r} AD'(r) + AD''(r) \right\} \end{aligned} \quad (5.10)$$

Multiplying by $\frac{h^2}{2}$ and substituting into (5.5):

$$\begin{aligned}
& \frac{\phi(r+h) - 2\phi(r) + \phi(r-h)}{h^2} + \frac{g}{r} \frac{\phi(r+h) - \phi(r-h)}{2h} - \delta \phi(r) \\
& + \frac{h^2}{12} \left(\frac{g^2}{r^2} - \frac{2g}{r^2} - \delta \right) \frac{\phi(r+h) - 2\phi(r) + \phi(r-h)}{h^2} + \frac{h^2}{12} \left[\frac{2g}{r^3} - \frac{g}{r} \left(\frac{g}{r^2} + \delta \right) \right] \frac{\phi(r+h) - \phi(r-h)}{2h} \\
& + \frac{h^2}{12} \frac{B(r+2h) - 2B(r+h) + 2B(r-h) - B(r-2h)}{2h^3} + \frac{h^2}{12} \frac{2g}{r} \frac{B(r+h) - 2B(r) + B(r-h)}{h^2} \\
& + \frac{h^2}{12} \left(\frac{g^2}{r^2} - \frac{2g}{r^2} \right) \frac{B(r+h) - B(r-h)}{2h} + \frac{h^2}{12} \left(\frac{2g}{r^3} - \frac{g^2}{r^3} \right) B(r) \\
& + \frac{h^2}{12} \frac{g}{r} A \frac{D(r+h) - D(r-h)}{2h} + \frac{h^2}{12} A \frac{D(r+h) - 2D(r) + D(r-h)}{h^2} + \frac{B(r+h) - B(r-h)}{2h} \\
& + \frac{g}{r} B(r) - \frac{h^2}{6} \frac{B(r+2h) - 2B(r+h) + 2B(r-h) - B(r-2h)}{2h^3} + AD(r) = 0
\end{aligned} \tag{5.11}$$

Collecting terms, multiplying by $\frac{h^2}{2}$:

$$\begin{aligned}
& \phi(r+h) \left\{ \frac{1}{2} + \frac{gh}{4r} + \frac{g(g-2)}{24} \frac{h^2}{r} - \frac{g(g-2)}{48} \frac{h^3}{r^3} - \frac{\delta h^2}{24} + \frac{g\delta h^3}{48r} \right\} \\
& - \phi(r) \left\{ 1 + \frac{g(g-2)}{12r^2} h^2 + \frac{5\delta h^2}{12} \right\} \\
& + \phi(r-h) \left\{ \frac{1}{2} - \frac{gh}{4r} + \frac{g(g-2)}{24r^2} h^2 + \frac{g(g-2)}{48r^3} h^3 - \frac{\delta h^2}{24} + \frac{g\delta h^3}{48r} \right\} \\
& + B(r+2h) \left(\frac{h}{48} - \frac{h}{24} \right) \\
& + B(r+h) \left\{ \frac{h^2}{12} \frac{g}{r} - \frac{h}{24} + \frac{h^3}{48} \left(\frac{g^2}{r^2} - \frac{2g}{r^2} \right) + \frac{h}{4} + \frac{h}{12} \right\} \\
& + B(r) \left\{ \frac{h^4}{24} \left(\frac{2g}{r^3} - \frac{g^2}{r^3} \right) - \frac{h^2}{6} \frac{g}{r} + \frac{h^2}{2} \frac{g}{r} \right\} \\
& + B(r-h) \left\{ \frac{h}{24} + \frac{h^2}{12} \frac{g}{r} - \frac{h^3}{48} \left(\frac{g^2}{r^2} - \frac{2g}{r^2} \right) - \frac{h}{4} - \frac{h}{12} \right\} \\
& + B(r-2h) \left(\frac{h}{24} - \frac{h}{48} \right) \\
& + AD(r+h) \left\{ \frac{h^3}{48} \frac{g}{r} + \frac{h^2}{24} \right\} \\
& + AD(r) \left\{ \frac{h^2}{2} - \frac{h^2}{12} \right\} \\
& + AD(r-h) \left\{ \frac{h^2}{24} - \frac{h^3}{48} \frac{g}{r} \right\} = 0
\end{aligned} \tag{5.12}$$

(5.12) may be written as the difference equation

$$P_K \Omega_{K+1} - Q_K \Omega_K + R_K \Omega_{K-1} + S_K = 0 \quad (5.13)$$

where

$$\begin{aligned} \Omega_K &= \text{Flux at space point } K \\ P_K &= \frac{1}{2} + \frac{g h}{4r} + \frac{g(g-2)}{24} \frac{h^2}{r^2} - \frac{g(g-2)}{48} \frac{h^3}{r^3} - \frac{5 h^2}{24} + \frac{5 h^3 g}{48 r} \\ Q_K &= 1 + \frac{g(g-2)}{12} \frac{h^2}{r^2} + \frac{55 h^2}{12} \\ R_K &= \frac{1}{2} - \frac{g h}{4r} + \frac{g(g-2)}{24} \frac{h^2}{r^2} + \frac{g(g-2) h^3}{48 r^3} - \frac{5 h^2}{24} + \frac{5 h^3}{48 r} \\ S_K &= -\frac{h}{48} B(r+2h) + \left[\frac{2}{24} h + \frac{h^2}{12} \frac{g}{r} \left\{ 1 + \frac{h}{r} (g-2) \right\} \right] B(r+h) \\ &\quad + \frac{h^2}{2} \frac{g}{r} \left\{ \frac{2}{3} + \frac{h^2}{12 r^2} (2-g) \right\} B(r) + \left\{ -\frac{2}{24} h + \frac{h^2}{12} \frac{g}{r} \left[1 - \frac{h}{4r} (g-2) \right] \right\} B(r-h) \\ &\quad + \frac{h}{48} B(r-2h) + A \left\{ \frac{h^2}{24} \left(\frac{h}{2} \frac{g}{r} + 1 \right) D(r+h) + \frac{5 h^2}{12} D(r) \right. \\ &\quad \left. + \frac{h^2}{24} \left(1 - \frac{h}{2} \frac{g}{r} \right) D(r-h) \right\} \end{aligned} \quad (5.14)$$

B. Boundary Conditions at Shells

Equation (3.33), discarding bits of notation unnecessary for this discussion, is

$$\phi_i(r) = -\frac{1}{A} \left\{ \phi'_0(r) + B(r) \right\} \quad (5.15)$$

now

(5.16)

$$j_{\pm}(r) = \frac{1}{4} \phi_0(r) \mp \frac{1}{2A} \left\{ \phi_0'(r) + B(r) \right\}$$

where

$j_{\pm}(r)$ = Partial current in the $\left\{ \begin{smallmatrix} + \\ - \end{smallmatrix} \right\}$ direction

The following expressions were developed⁽¹⁾ for exit currents

from a shell due to j_{+} impinging:

Forward exit current:

$$\frac{P^1}{4} \phi_0(r) - \frac{Q^1}{2A} \left\{ \phi_0'(r) + B(r) \right\}$$

(5.17)

Backward exit current:

$$\frac{R^1}{4} \phi_0(r) - \frac{S^1}{2A} \left\{ \phi_0'(r) + B(r) \right\}$$

Figure 1
Shell Boundaries

A shell is represented as shown in Figure 1. The boundary conditions are

$$I^{\pm} \left\{ \frac{\phi_0(I)}{4} + \frac{1}{2A_I} [\phi_0'(I) + B(I)] \right\} = I^{\mp} \left\{ \frac{R^1 \phi_0(I)}{4} - \frac{S^1}{2A_I} [\phi_0'(I) + B(I)] \right\}$$

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$$+ J^2 \left\{ \frac{P^2 \phi_o(J)}{4} + \frac{Q^2}{2A_J} [\phi_o'(J) + B(J)] \right\}$$

$$J^2 \left\{ \frac{\phi_o(J)}{4} - \frac{1}{2A_J} [\phi_o'(J) + B(J)] \right\} = J^2 \left\{ \frac{R^2 \phi_o(J)}{4} + \frac{S^2}{2A_J} [\phi_o'(J) + B(J)] \right\} \quad (5.18)$$

$$+ I^2 \left\{ \frac{P^2 \phi_o(I)}{4} - \frac{Q^2}{2A_I} [\phi_o'(I) + B(I)] \right\}$$

or

$$\left. \begin{aligned} I^2 \left\{ R \phi_o(I) + \frac{2S}{A_I} [\phi_o'(I) + B(I)] \right\} &= J^2 \left\{ \frac{P \phi_o(J)}{4} + \frac{2Q}{A_J} [\phi_o'(J) + B(J)] \right\} & (a) \\ I^2 \left\{ P \phi_o(I) - \frac{2Q}{A_I} [\phi_o'(I) + B(I)] \right\} &= J^2 \left\{ R \phi_o(J) - \frac{2S}{A_J} [\phi_o'(J) + B(J)] \right\} & (b) \end{aligned} \right\} \quad (5.19)$$

where

$$\left. \begin{aligned} P &= P^2 \\ Q &= Q^2 \\ R &= 1 - R^2 \\ S &= 1 + S^2 \end{aligned} \right\} \quad (5.20)$$

Multiplying (5.19,a) by R and subtracting (5.19,b) $\times P$,

multiplying (5.19,a) by S and subtracting (5.19,b) $\times Q$,

and defining

$$\begin{aligned} 2\beta_1 &= PS + RQ \\ 2\beta_2 &= RS + PQ \\ 2\beta_3 &= S^2 - Q^2 \\ 2\beta_4 &= R^2 - P^2 \end{aligned} \quad (5.21)$$

puts (5.19) into the form

$$\left. \begin{aligned} \beta_4 \phi_o(I) + \frac{2\beta_2}{A_I} [\phi_o'(I) + B(I)] &= \left(\frac{J}{I} \right)^2 \frac{2\beta_1}{A_J} [\phi_o'(J) + B(J)] \\ \beta_2 \phi_o(I) + \frac{2\beta_3}{A_I} [\phi_o'(I) + B(I)] &= \left(\frac{J}{I} \right)^2 \beta_1 \phi_o(J) \end{aligned} \right\} \quad (5.22)$$

From (5.4) and (5.7)

$$\begin{aligned}\phi'(r) &= \frac{\phi(r+h) - \phi(r-h)}{2h} + \frac{h^2}{6} \left\{ \frac{g}{r} \phi''(r) - \left(\frac{g}{r^2} + S \right) \phi'(r) + B''(r) \right. \\ &\quad \left. + \frac{g}{r} B'(r) - \frac{g}{r^2} B(r) + A D'(r) \right\} \\ \phi'(r) &= \frac{\phi(r+h) - \phi(r-h)}{2h} + \frac{h^2}{6} \frac{g}{r} \frac{\phi(r+h) - 2\phi(r) + \phi(r-h)}{h^2} \quad (5.23) \\ &\quad - \frac{h^2}{6} \left(\frac{g}{r^2} + S \right) \frac{\phi(r+h) - \phi(r-h)}{2h} + \frac{h^2}{6} \frac{B(r+h) - 2B(r) + B(r-h)}{h^2} \\ &\quad + \frac{g}{r} \frac{h^2}{6} \frac{B(r+h) - B(r-h)}{2h} - \frac{h^2}{6} \frac{g}{r^2} B(r) + \frac{A h^2}{6} \frac{D(r+h) - D(r-h)}{2h}\end{aligned}$$

Collecting terms and reducing

$$\begin{aligned}\phi'(r) &= \frac{\phi(r+h)}{h} \left\{ \frac{1}{2} + \frac{g}{6} \frac{h}{r} - \frac{g}{12} \frac{h^2}{r^2} - \frac{S h^2}{12} \right\} - \frac{1}{3} \frac{g h}{r} \frac{\phi(r)}{h} \\ &\quad + \frac{\phi(r-h)}{h} \left\{ \frac{g h}{6 r} - \frac{1}{2} + \frac{g h^2}{2 r^2} + \frac{S h^2}{12} \right\} \\ &\quad + B(r+h) \left\{ \frac{1}{6} + \frac{g}{12} \frac{h}{r} \right\} \\ &\quad + B(r) \left\{ -\frac{1}{3} - \frac{g}{6} \frac{h^2}{r^2} \right\} \\ &\quad + B(r-h) \left\{ \frac{1}{6} - \frac{g}{12} \frac{h}{r} \right\} \\ &\quad + \frac{A h}{12} \{ D(r+h) - D(r-h) \} \quad (5.24)\end{aligned}$$

say

$$\phi'(r) = M \phi(r+h) + N \phi(r) + L \phi(r-h) + X(r) \quad (5.25)$$

where

$$\begin{aligned}
 M &= \frac{1}{h} \left\{ \frac{1}{2} + \frac{gh}{6r} - \frac{1}{12} \left(\frac{gh^2}{r^2} + gh^2 \right) \right\} \\
 N &= - \left\{ \frac{1}{3} \frac{gh}{r} \right\} \frac{1}{h} \\
 L &= \frac{1}{h} \left\{ -\frac{1}{2} + \frac{gh}{6r} + \frac{1}{12} \left(\frac{gh^2}{r^2} + gh^2 \right) \right\} \\
 X(r) &= \frac{1}{6} \left\{ 1 + \frac{g}{2} \frac{h}{r} \right\} B(r+h) - \frac{1}{3} \left\{ 1 + \frac{g}{2} \frac{h^2}{r^2} \right\} B(r) \\
 &\quad + \frac{1}{6} \left\{ 1 - \frac{g}{2} \frac{h}{r} \right\} B(r-h) + \frac{gh}{12} \left\{ D(r+h) - D(r-h) \right\}
 \end{aligned} \tag{5.26}$$

Substituting (5.25) into (5.22) and using difference notation:

$$\begin{aligned}
 \beta_1 \Omega_I + \frac{2\beta_2}{A_I} [M_I \Omega_{I+1} + N_I \Omega_I + L_I \Omega_{I-1} + X + B(I)] &= \\
 = Y \frac{2\beta_1}{A_J} [M_J \Omega_{J+1} + N_J \Omega_J + L_J \Omega_{J-1} + X_J + B(J)] & \\
 \beta_2 \Omega_I + \frac{2\beta_3}{A_I} [M_I \Omega_{I+1} + N_I \Omega_I + L_I \Omega_{I-1} + X + B(I)] &= \\
 = Y \beta_1 \Omega_J &
 \end{aligned} \tag{5.27}$$

where $Y = \left(\frac{I}{J} \right)^g$

Defining $\chi^*(I) = X(I) + B(I)$

(5.27) become

$$\begin{aligned}
 \frac{2\beta_2}{A_I} M_I \Omega_{I+1} + (\beta_1 + \frac{2\beta_2}{A_I} N_I) \Omega_I + \frac{2\beta_2}{A_I} L_I \Omega_{I-1} + \frac{2\beta_2}{A_I} \chi_I^* &= \\
 = Y \frac{2\beta_1}{A_J} \left\{ M_J \Omega_{J+1} + N_J \Omega_J + L_J \Omega_{J-1} + \chi_J^* \right\} & \\
 \frac{2\beta_3}{A_I} M_I \Omega_{I+1} + (\beta_2 + \frac{2\beta_3}{A_I} N_I) \Omega_I + \frac{2\beta_3}{A_I} L_I \Omega_{I-1} + \frac{2\beta_3}{A_I} \chi_I^* &= Y \beta_1 \Omega_J
 \end{aligned} \tag{5.28}$$

It is evident some fictitious points are needed in a shell since the derivative is needed at I and J. The sequence of points is illustrated in Figure 2.

Figure 2
Sequence of Space Points

Writing, now, (5.13) at I and at J:

$$\left. \begin{aligned} P_I \Omega_{I+1} - Q_I \Omega_I + R_I \Omega_{I-1} + S_I &= 0 \\ P_J \Omega_{J+1} - Q_J \Omega_J + R_J \Omega_{J-1} + S_J &= 0 \end{aligned} \right\} \quad (5.29)$$

If Ω_{I-1} , Ω_J and Ω_{J+1} are eliminated from (5.28) and (5.29) an equation is obtained of the form

$$P_{I+1} \Omega_I - Q_{I+1} \Omega_{I+1} + R_{I+1} \Omega_{I-1} + S_{I+1} = 0 \quad (5.30)$$

with coefficients

$$\left. \begin{aligned} P_{I+1} &= 2\gamma R_I (R_J M_J - P_J L_J) \beta_1 A_I \\ Q_{I+1} &= -2(R_I M_I - P_I L_I) \left\{ \beta_2 P_J A_J - 2\beta_3 (Q_J M_J + P_J N_J) \right\} \\ R_{I+1} &= A_I A_J R_I P_J \beta_4 - 2\beta_2 \left\{ R_I A_I (M_J Q_J + P_J N_J) \right. \\ &\quad \left. - P_J A_J (Q_I L_I + R_I N_I) \right\} - 4\beta_3 (Q_I L_I + R_I N_I) (M_J Q_J + P_J N_J) \\ S_{I+1} &= R_I P_J \left\{ 2\beta_2 A_J W_I - 2\beta_3 A_I W_J Y \right\} - 4R_I W_I \beta_3 (P_J N_J + M_J Q_J) \\ W_I &= \chi_I^* - \frac{L_I S_I}{R_I} \\ W_J &= \chi_J^* - \frac{M_J S_J}{P_J} \end{aligned} \right\} \quad (5.31)$$

Elimination of Ω_{I-1} , Ω_I , and Ω_{J+1} from (5.28) and (5.29) yields an equation of the form

$$P_{J-1} \Omega_{I+1} - Q_{J-1} \Omega_{J-1} + R_{J-1} \Omega_J + S_{J-1} = 0 \quad (5.32)$$

where

$$\begin{aligned} P_{J-1} &= -R_{I+1} \\ Q_{J-1} &= 2(R_J M_J - L_J P_J) \left\{ A_I R_I \beta_2 + 2\beta_3 (R_I N_I + Q_I L_I) \right\} \\ R_{J-1} &= -\frac{2}{Y} P_J \beta_1 A_J (R_I M_I - P_I L_I) \\ S_{J-1} &= 2 P_J R_I \left\{ -\beta_1 A_J W_I \frac{1}{Y} + A_I \beta_2 W_J \right\} + 4 P_J \beta_3 W_J (R_I N_I + Q_I L_I) \end{aligned} \quad (5.33)$$

If there is no shell

$$\begin{aligned} \beta_1 &= \beta_2 = 1 \\ \beta_3 &= \beta_4 = 0 \\ Y &= 1 \end{aligned} \quad (5.34)$$

and (5.31) and (5.33) reduce to

$$\begin{aligned} Q_{J-1} &= P_{I+1} = 2 R_I (R_J M_J - P_J L_J) A_I \\ R_{J-1} &= Q_{I+1} = -2 (R_I M_I - P_I L_I) P_J A_J \\ -P_{J-1} &= R_{I+1} = 2 \left\{ P_J A_J (Q_I L_I + R_I N_I) - R_I A_I (M_J Q_J + P_J N_J) \right\} \\ -S_{J-1} &= S_{I+1} = R_I P_J \left\{ 2 A_J W_I - 2 A_I W_J \right\} \end{aligned} \quad (5.35)$$

C. Γ, Δ Method of Integration

It is convenient in the satisfaction of the boundary conditions at the origin and outside boundary to say

$$\Omega_K = \Gamma_K \Omega_{K+1} + \Delta_K \quad (5.36)$$

Substitution into (5.13) shows

$$\begin{aligned} \Gamma_K &= \frac{P_K}{Q_K - R_K \Gamma_{K-1}} \\ \Delta_K &= \frac{R_K \Delta_{K-1} + S_K}{Q_K - R_K \Gamma_{K-1}} \end{aligned} \quad (5.37)$$

D. Boundary Condition at the Origin

The differential equation is

$$\phi''(r) + \frac{q}{r} \phi'(r) - \delta \phi(r) + B'(r) + \frac{q}{r} B(r) + AD(r) = 0 \quad (5.38)$$

Expanding these functions about 0 and collecting coefficients of like powers of r :

$$\text{for } r^{-1}: q \phi'(0) + q B(0) = 0$$

$$r^0: \phi''(0)(1+q) - \delta \phi(0) + (1+q) B'(0) + AD(0) = 0$$

$$r^1: \phi'''(0) \left\{1 + \frac{q}{2}\right\} - \delta \phi'(0) + B''(0) \left(1 + \frac{q}{2}\right) + AD'(0) = 0 \quad (5.39)$$

$$r^2: \phi^{IV}(0) \left(1 + \frac{q}{3}\right) - \delta \phi''(0) + B'''(0) \left(1 + \frac{q}{3}\right) + AD''(0) = 0$$

Note that ϕ_1 is an odd function and B goes as ϕ_1 , while ϕ_0 is even and D goes as ϕ_0 .

$$\text{from (5.39), } r^{-1}, B(0) = 0$$

From (5.39) r^0 :

$$\phi''(0)(1+q) - \delta \phi(0) + (1+q) B'(0) + AD(0) = 0 \quad (5.40)$$

from (5.39), r^1 :

$$\phi'''(0) = B'''(0) = 0 \quad (5.41)$$

from (5.39), r^2 :

$$\phi^{IV}(0) = \frac{\delta}{1 + \frac{q}{3}} \phi''(0) - B'''(0) - \frac{A}{1 + \frac{q}{3}} D''(0) \quad (5.42)$$

Replacing derivatives in (5.40) by their difference approximations from

(5.4):

$$\begin{aligned} & (1+q) \left\{ \frac{\phi(r+h) - 2\phi(r) + \phi(r-h)}{h^2} - \frac{h^2}{12} \phi^{IV}(r) \right\}_{r=0} - \delta \phi(0) \\ & + (1+q) \left\{ \frac{B(r+h) - B(r-h)}{2h} - \frac{h^2}{6} B'''(r) \right\}_{r=0} + AD(0) = 0 \end{aligned} \quad (5.43)$$

Substituting from (5.42) and recalling

$$\phi(r) = \phi(-r)$$

$$B(r) = -B(-r)$$

(5.44)

$$\begin{aligned} (1+g) \left\{ \frac{2}{h^2} [\phi(h) - \phi(0)] - \frac{h^2}{12} \left[\frac{S}{1+\frac{g}{3}} \frac{2}{h^2} [\phi(h) - \phi(0)] \right. \right. \\ \left. \left. - \frac{B(2h) - 2B(h)}{h^3} - \frac{A}{1+\frac{g}{3}} \frac{2}{h^2} [D(h) - D(0)] - S \phi(0) \right] \right. \\ \left. + (1+g) \left\{ \frac{B(h)}{h} - \frac{h^2}{6} \frac{B(2h) - 2B(h)}{h^3} \right\} + AD(0) \right\} = 0 \end{aligned} \quad (5.45)$$

Collecting terms

$$\begin{aligned} \phi(h) \left\{ \frac{2(1+g)}{h^2} - \frac{S(1+g)}{6(1+\frac{g}{3})} \right\} - \phi(0) \left\{ \frac{2(1+g)}{h^2} - \frac{S(1+g)}{6(1+\frac{g}{3})} + S \right\} \\ - B(2h) \left\{ -\frac{1+g}{12h} + \frac{(1+g)}{6h} \right\} + B(h) \left\{ \frac{1+g}{3h} - \frac{1+g}{6h} + \frac{1+g}{h} \right\} \\ + D(h) \frac{2A(1+g)}{12(1+\frac{g}{3})h^2} + AD(0) \left\{ 1 - \frac{2(1+g)}{12h^2(1+\frac{g}{3})} \right\} = 0 \end{aligned} \quad (5.46)$$

so

$$\begin{aligned} \phi(0) &= \Gamma_0 \phi(h) + \Delta_0 \\ \Omega_0 &= \Gamma_0 \Omega_1 + \Delta_0 \end{aligned} \quad (5.47)$$

where

$$\begin{aligned} \Gamma_0 &= \frac{\left\{ 1 - \frac{S h^2}{4(3+g)} \right\} (1+g)}{\left\{ 1 - \frac{S h^2}{4(3+g)} \right\} (1+g) + \frac{S h^2}{2}} \\ \Delta_0 &= \frac{(1+g) \frac{h}{12} \left\{ 7B(h) - \frac{B(2h)}{2} \right\} + \frac{h^2 A}{4(3+g)} \left\{ (1+g) D(h) + (5+g) D(0) \right\}}{\left[1 - \frac{S h^2}{4(3+g)} \right] (1+g) + \frac{S h^2}{2}} \end{aligned} \quad (5.48)$$

E. Boundary Condition at Outside Boundary

The boundary condition at the outside boundary is

$$\begin{aligned} j^-(N) &= \text{backward exit current} \\ N &= \text{outside boundary} \end{aligned} \quad (5.49)$$

that is

$$\frac{1}{4} \phi(N) + \frac{1}{2A_N} \left\{ \phi'(N) + B(N) \right\} = \frac{R^2 \phi(N)}{4} - \frac{S^2}{2A_N} \left\{ \phi'(N) + B(N) \right\} \quad (5.50)$$

or
$$R \phi(N) + \frac{2S}{A_N} \left\{ \phi'(N) + B(N) \right\} = 0 \quad (5.51)$$

Define
$$\beta_S = \frac{S}{R} \quad (5.52)$$

Then
$$\phi(N) + \frac{2\beta_S}{A_N} \left\{ \phi'(N) + B(N) \right\} = 0 \quad (5.53)$$

Substitute from (5.25) and change to difference notation

$$\Omega_N + \frac{2\beta_S}{A_N} \left\{ M_N \Omega_{N+1} + N_N \Omega_N + L_N \Omega_{N-1} + \chi_N^* \right\} = 0 \quad (5.54)$$

Substituting from (5.36) leads to

$$\Omega_{N+1} = - \frac{2\beta_S \chi_N^* + \Delta_N \left\{ A_N + 2\beta_S \left[\frac{L_N \Delta_{N-1}}{\Delta_N} + N_N + L_N \Gamma_{N-1} \right] \right\}}{2\beta_S M_N + \Gamma_N \left\{ A_N + 2\beta_S [N_N + L_N \Gamma_{N-1}] \right\}} \quad (5.55)$$

F. Sequence of Steps in Spatial Integration

The boundary condition at the origin is satisfied in the calculation of Γ_0 and Δ_0 from equations (5.48). Equation (5.37) together with (5.31), (5.33), and (5.35) allow computation of the Γ_K and Δ_K to the outside boundary. Ω_{N+1} , the flux at a fictitious point outside the boundary, is computed from (5.55) and in so doing, the outside boundary condition is satisfied. Using (5.36), the flux at each space point may be calculated.

APPENDIX

Consider the case where the scattering process is azimuthally symmetric about the initial direction of motion of the neutron; i.e., isotropic scattering in the center of mass system. Define

$$J_n(u' \rightarrow u) du = \left(\begin{array}{l} \text{Probability that given a neutron with} \\ \text{lethargy } u' \text{ before a scattering colli-} \\ \text{sion, the lethargy of the neutron after} \\ \text{collision will be in } du \text{ about } u. \end{array} \right)$$

Mathematically

$$J_n(u' \rightarrow u) = \begin{cases} 0 & u' > u \\ \frac{e^{u'-u}}{1-\alpha} & u' - \ln \alpha \geq u \geq u' \\ 0 & u > u' + \ln \alpha \end{cases} \quad (A-1)$$

Now from Section I, equation (1.9)

$$\int_u^\infty J_n(u' \rightarrow u'') du'' = \int_{u'}^{u' - \ln \alpha} \frac{e^{u'-u''}}{1-\alpha} du'' = 1 \quad (A-2)$$

For the case of P_1 scattering only in the center of mass system we define

$$K_n(u' \rightarrow u) = \left(\begin{array}{l} \text{Probability that given a neutron with} \\ \text{lethargy } u' \text{ before a scattering colli-} \\ \text{sion, the lethargy of the neutron after} \\ \text{collision will be in } du \text{ about } u. \end{array} \right)$$

This time

$$K_n(u' \rightarrow u) = \begin{cases} 0 & u' > u \\ J_n(u' \rightarrow u) \nu_0(u, u') & u' + \ln \alpha \geq u \geq u' \\ 0 & u > u' - \ln \alpha \end{cases}$$

where $\mu_0(u, u')$ is the cosine of the scattering angle and is given by

$$\mu_0(u, u') = \frac{1}{2} \left[(A+1) e^{\frac{1}{2}(u'-u)} - (A-1) e^{-\frac{1}{2}(u'-u)} \right]$$

$J_n(u' \rightarrow u)$ is defined by (A.1).

Evaluating

$$\int_u^\infty K_n(u \rightarrow u') du' = \int_u^\infty \frac{u' - \ln \alpha}{2(1-\alpha)} \left\{ (A+1) e^{\frac{1}{2}(u'-u)} - (A-1) e^{-\frac{1}{2}(u'-u)} \right\} du' \quad (A.4)$$

$$\int_u^\infty K_n(u \rightarrow u') du' = \frac{2}{3A_n}$$

We will now examine the constants ξ and η .

For ξ we have from page 5 of Section I

$$\xi_n = \int_0^u (u-u') J_n(u' \rightarrow u) du'$$

Substituting from (A.1)

$$\xi_n = \frac{1}{1-\alpha} \int_{u+\ln \alpha}^u (u-u') e^{u'-u} du' = 1 + \frac{a_n \ln \alpha_n}{1-\alpha_n} \quad (A.5)$$

where

$$\alpha = \left(\frac{A-1}{A+1} \right)^2$$

For values of A greater than 10, a good approximation to (A.5) is

$$\xi_n \approx \frac{2}{A + \frac{2}{3}}$$

Considering η_n we see from page 6, Section I

$$\eta_n = \int_0^u (u-u') K_n(u' \rightarrow u) du' = \frac{1}{2(1-\alpha_n)} \int_0^u \left\{ (u'-u) \left[(A_n+1) e^{\frac{1}{2}(u'-u)} - (A_n-1) e^{-\frac{1}{2}(u'-u)} \right] \right\} du' \quad (A.6)$$

$$= \frac{A+1}{2(\alpha_n-1)} \left\{ 4 \alpha_n^{\frac{1}{2}} (1-\alpha_n^{\frac{1}{2}}) - 2 \alpha_n \ln \alpha_n \left(\frac{\alpha_n^{\frac{1}{2}}}{3} - 1 \right) - \frac{4}{9} (1-\alpha_n^{\frac{3}{2}}) \right\}$$

In terms of A and ξ , (A.6) reduced to

$$\eta_n = \frac{12 A_n + 10}{9 A_n} - \frac{2}{3} \xi_n (A_n + 2)$$

The constants δ_n and ρ_n will now be reduced to more convenient form than given in Section I of the report. From (1.13)

$$\delta_n = - \frac{a_n}{\xi_n} = 1 - \frac{a_n \ln a_n}{\xi_n (1-a_n)}$$

Writing in terms of A and ξ while rearranging gives

$$\delta_n = 1 - \frac{2A_n}{\xi_n} \left(\frac{\xi_n - 1}{A_n - 1} \right)^2 \quad (\text{A.8})$$

From (1.18)

$$\rho_n = \frac{b_n}{\eta_n}$$

Noting (1.16) we have defined b_n as

$$b_n = \frac{A_n + 1}{2(1-a_n)} \left\{ 4a_n^{\frac{1}{2}} [2(a_n^{\frac{1}{2}} - 1) - a_n^{\frac{1}{2}} \ln a_n] - a_n \ln^2 a_n \left(\frac{a_n^{\frac{1}{2}}}{3} - 1 \right) - \frac{4}{9} \left[\frac{2}{3} (a_n^{\frac{1}{2}} - 1) - a_n^{\frac{1}{2}} \ln a_n \right] \right\}$$

By introducing a in terms of A and noting the value of ξ and δ we are able to express b_n as

$$b_n = \frac{4(15A_n + 14)}{27A_n} - \frac{2}{9} \xi_n (5A_n + 4) - \frac{2}{3} \xi_n \delta_n (A_n + 2) \quad (\text{A.9})$$

Summarizing $\int_u^\infty \mathcal{I}_n(u' \rightarrow u'') du'' = 1$

$$\int_u^\infty \kappa_n(u \rightarrow u') du' = \frac{2}{3A_n}$$

$$\xi_n = 1 + \frac{a_n \ln a_n}{1 - a_n} \approx \frac{2}{A_n + \frac{2}{3}}$$

$$\eta_n = \frac{12A_n + 10}{9A_n} - \frac{2}{3} \xi_n (A_n + 2)$$

$$\delta_n = \frac{a_n}{\xi_n} = 1 - \frac{2A_n}{\xi_n} \left(\frac{\xi_n - 1}{A_n - 1} \right)^2$$

$$\rho_n = \frac{b_n}{\eta_n} ; \text{ where } b_n \text{ is given by (A.9)}$$